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HERMES : A PERSONAL-COMPUTER PROGRAM FOR CALCULATION  
OF THE FERMI-GAS MODEL PARAMETERS  
OF NUCLEAR LEVEL DENSITY

September 1993

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HERMES: A Personal-computer Program for Calculation of  
the Fermi-gas Model Parameters of Nuclear Level Density

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A computer program, HERMES, that provides the quantities usually needed in nuclear level density calculations, has been developed. The applied model is the standard Fermi Gas Model (FGM) in which pairing correlations and shell effects are opportunely taken into account. The effects of additional nuclear structure properties together with their inclusion into the computer program are also considered. Using HERMES, a level density parameter systematics has been constructed for mass range  $41 \leq A \leq 253$ .

**Keywords:** Fermi-gas Model, Nuclear Level Density, Level Density Parameters, Level Density Parameter Systematics, Pairing Correlations, Shell-effects

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H E R M E S : 原子核準位密度のフェルミガス模型パラメータ計算のための  
パーソナルコンピューター用プログラム

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(1993年8月24日受理)

原子核の準位密度計算に通常必要とされる物理量を計算するプログラム H E R M E S を開発した。核内核子の対相関と殻効果を取り入れた標準のフェルミガス模型をモデルとして用いた。その他の原子核構造の性質の効果のプログラムへの組み込みについても議論した。H E R M E S を用いて質量が41から253までの質量領域において準位密度パラメータの系統式を作成した。

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## 1. INTRODUCTION

The calculation of nuclear level densities at excitation energies of a few MeV can be performed using the Fermi-Gas model (FGM). A certain number of modifications of the basic FGM are necessary in order to take into account nuclear properties of various nature. For example, corrections due to pairing correlations and shell inhomogeneities have to be incorporated to provide a realistic description of nuclear excitations.

On the other hand, an important, experimentally reachable quantity which allows for testing nuclear models employed in level density calculation is the average spacings of s-wave neutron resonances,  $\langle D \rangle_{l=0}$ . A large set of information on this quantity has been collected and compiled several times in the past. A relatively recent compilation<sup>1)</sup> has been made available which provides a large data-base on which the traditional level density models can be tested.

We have coded the FGM prescriptions into a computer program, HERMES, which provides the nuclear level density parameters based on fundamental nuclear structure information and on the experimental average spacings of s-wave neutron resonances. The program has been written in order to provide the user with the basic parameters usually employed in level density calculations. The parameters supplied by HERMES should be largely compatible with the parametrization adopted, for example, in codes using the Hauser-Feshbach statistical theory for the calculation of nuclear cross sections. HERMES has been made to be run on personal computers. It would be, however, trivial to separate and include its basic components into any larger code for nuclear reaction calculations.

The details of our model description with some discussions on the various nuclear structure effects included into the FGM are given in our previous paper<sup>2)</sup>. Here we will limit ourselves to give the definition of the basic quantities for nuclear level density calculation and we will then describe the computer program. Finally, examples will be presented to show the capabilities of the use of HERMES.

The program, together with the data-base files are available upon request to the authors (see the request-form in the Appendix).

## 2. BASIC RELATIONS FOR THE NUCLEAR LEVEL DENSITY DESCRIPTION

### 2.1 The Fermi-Gas model

The state-density for a set of  $A$  non-interacting nucleons ( $Z$  protons and  $N$  neutrons) arranged on a single-particle spectrum with spacing  $g_f$  at the fermi energy can be easily derived to give<sup>3)</sup>

$$\rho_{Z,N}(U) = \frac{\sqrt{\pi}}{12 a^{1/4} U^{5/4}} e^{2\sqrt{aU}} \quad (1)$$

where  $U$  is the available excitation energy and  $a \equiv (\pi^2/6)g_f^2$  is a level density parameter.

The density of nuclear levels, i.e. states of given total angular momentum  $J$  and fixed parity  $\Pi$  is given by

$$\rho_{Z,N}(U,J,\Pi) = \rho_{Z,N}(U) f_\sigma(J) g_{par}(\Pi) \quad (2)$$

where  $f_\sigma(J)$  can be derived by differentiating respect to state with  $M = J$  and  $M = J + 1$  a gaussian distribution for the projection of the total angular momentum,  $M$ , with dispersion  $\sigma$ :

$$f_\sigma(J) = \frac{2J+1}{2\sigma^2 \sqrt{2\pi\sigma^2}} e^{-\frac{J(J+1)}{2\sigma^2}} \quad (3)$$

and  $g_{par}(\Pi)$  is a function describing the parity distribution.

Nuclear energy levels have a clearly unsymmetrical parity distribution in the lower part of the spectrum. As the excitation energy increases, however, the number (or density) of levels with opposite parity tends to be the same. Except for some light nuclei, the parity distribution at excitation energies corresponding to the neutron separation energy can be assumed to be symmetrical. To treat the cases in which the parity distribution is asymmetrical some technique has been proposed<sup>4)</sup>. The possibility of including this effect has been analyzed in several practical applications but a systematic analysis on a large mass range has not yet been done. For this reason the commonly adopted assumption of equal probability for different parity states has been adopted in the present analysis:

$$g_{par}(\Pi) = \frac{1}{2}. \quad (4)$$

In addition to the parameter  $a$ , the only other quantity to be determined in Eq. (2) is the spin dispersion factor  $\sigma$ . For a gas of fermions constrained into a spherical box of radius  $R$ , the dispersion factor  $\sigma$  can be evaluated to give

$$\sigma^2 = \frac{2}{5} (M_n R^2/\hbar^2) A T \quad (5)$$

where  $M_n$  is the nucleon mass and  $T$  the nuclear temperature in MeV units. This is equivalent to consider the rotation of a rigid body with moment of inertia

$$I_r = \frac{2}{5} A M_n R^2 \quad (6)$$

which furnishes

$$\sigma^2 = \frac{I_r}{\hbar^2} T = 0.01389 A^{5/3} T \quad (7)$$

when using  $R = 1.2 A^{1/3}$  fm and  $M_n = 938.926$  MeV.

If the condition of spherical symmetry is released, the moments of inertia for an axially symmetric deformed rigid body with deformation  $\epsilon$  become

$$I_{\perp} = I_r (1 + \frac{1}{3} \epsilon) \quad (8)$$

and

$$I_{\parallel} = I_r (1 - \frac{2}{3} \epsilon) \quad (9)$$

for rotations perpendicular and parallel to the symmetry axis (Eq. (8) and Eq. (9) respectively). In this case the spin dispersion factor becomes

$$\sigma^2 = \frac{I_{\perp}^{2/3} I_{\parallel}^{1/3}}{\hbar^2} T \quad (10)$$

In the equations above, the nuclear deformation  $\epsilon$  is a parameter related to the nuclear quadrupole deformation by  $\epsilon = 0.945 \beta_2$ .

In the thermodynamical approach, the nuclear temperature is defined by the relation

$$\frac{1}{T} \equiv \frac{1}{\rho} \frac{d\rho}{dU} \quad (11)$$

For the Fermi-Gas, the relation

$$U = a T^2 \quad (12)$$

is usually adopted for defining the nuclear temperature. It is however straightforward to derive the value of the temperature from the state-density of Eq. (1):

$$\frac{1}{T} = \frac{1}{\sqrt{U/a}} - \frac{5}{4U}. \quad (13)$$

## 2.2 Pairing and shell-effects

The calculation of the level density using Eq. (2) is affected by the assumptions made when deriving the state-density from the thermodynamical equilibrium conditions (saddle-point inversion method, continuous approximation) as well as from the assumptions underlying the FGM itself. Quite generally the assumptions made in deriving Eq. (2) are well justified for excitation energies of a few MeV. In particular those approximations are generally valid for excitation energies corresponding to the neutron binding energy. This is an important point because at that energy the density of nuclear states of given  $J$  and  $\Pi$  is known from the spacing of neutron resonances (usually s-wave neutron resonances). In these cases it is possible to evaluate the only parameter of Eq. (2),  $a$ , from

$$\langle D \rangle_{l=0} = \frac{1}{\rho_{Z,N}(U, J=1/2, \Pi)} \quad (14)$$

for nuclei with  $I_\alpha = 0$ , or

$$\langle D \rangle_{l=0} = \frac{1}{\rho_{Z,N}(U, J=I_\alpha + 1/2, \Pi) + \rho_{Z,N}(U, J=I_\alpha - 1/2, \Pi)} \quad (15)$$

for nuclei with  $I_\alpha \neq 0$ , where  $I_\alpha$  is the spin of the nucleus with  $Z$  protons and  $N-1$  neutrons (target nucleus in the neutron + ( $Z$ ,  $N-1$ ) process). From the experimental  $\langle D \rangle_{l=0}^{\text{exp}}$  it is possible to derive the systematics of the level density parameter  $a$ .

The level density parameter  $a$  thus determined shows strong fluctuations over the entire mass range, essentially due to paring correlations and shell inhomogeneities (see Fig. 2 below).

A full treatment of the pairing correlation in nuclear motion may be based on statistical as well as on BCS theories<sup>5)</sup>. However, a much simpler but effective treatment of this effect can be incorporated into the model description simply redefining the excitation energy of the Fermi-Gas according to

$$\begin{aligned} U \rightarrow U - \delta & \quad \text{where } \delta = 2\Delta \quad \text{for even-even nuclei} \\ & = \Delta \quad \text{for odd nuclei} \\ & = 0 \quad \text{for odd-odd nuclei.} \end{aligned} \quad (16)$$

The pairing correlation parameter,  $\Delta$ , may be derived from mass-differences of neighboring nuclei for the entire mass region. However, the values derived from the experimental nuclear masses may be well represented by a simple, smooth function of the mass number. For example the value<sup>6)</sup>

$$\Delta = \frac{12}{\sqrt{A}} \quad (17)$$

has shown to be suitable for representing the experimental situation.

The use of this simple prescription may well be questioned from theoretical point of view since the relation (17) has been derived from even-odd difference in nuclear masses, i.e. at zero temperature. The situation may be different at finite temperature. However, using this simple procedure we have obtained good results as far as the level density parameter systematics is concerned (see below).

The inclusion of shell effects into the FGM description has been carried out using different approaches in the past. In our analysis we have adopted a technique due to Ignatyuk and coworkers<sup>7)</sup>. In this approach the level density parameter  $a$  depends on the excitation energy as well as on the shell correction energy  $E_{sh}$ :

$$a(U) = a(*) [ 1 + \frac{E_{sh}}{U} (1 - e^{-\gamma U}) ] \quad (18)$$

where  $a(*)$  is the asymptotic level density parameter to which  $a(U)$  tends for high excitation energies and  $\gamma$  a damping parameter.

The shell correction energy  $E_{sh}$  is defined as the difference between the experimental nuclear mass and a smooth theoretical mass value,  $M_w$ , derivable, for example, from a liquid-drop model:

$$E_{sh} \equiv M_{exp} - M_w . \quad (19)$$

The evaluation of this quantity requires some care because different liquid-drop model parametrizations are available from literature and they produce quite different values for  $E_{sh}$ .

Following this approach, for each isotope, the level density parameter  $a(*)$  is to be determined from the average neutron resonance spacing. In fact, the shell correction energy can be evaluated using Eq. (19) and the corresponding level density parameter  $a$  can be adjusted to fit the experimental  $\langle D \rangle_{l=0}^{exp}$  by varying  $a(*)$ .

### 2.3 Inclusion of other nuclear structure effects

The contribution of collective degrees of freedom in nuclear excitations is very important and different techniques have been proposed for its inclusion into the Fermi-Gas description. It is possible to show<sup>8)</sup> that the contribution of collective excitations to the state-density can be factorized into the form

$$\rho_{Z,N}(U) = \rho_{Z,N}^i(U) Z_{coll} \quad (20)$$

where  $Z_{coll}$  is the partition function for the collective degrees of freedom of the system with excitation energies  $E_c$

$$Z_{coll} = \sum_c e^{-\frac{E_c}{T}} \quad (21)$$

and  $\rho_{N,Z}^i(U)$  is the state density for the intrinsic (non-collective) excitations.

Various models have been employed in the past to evaluate the contribution of collective degrees of freedom to nuclear excitations<sup>6,7)</sup>. In the case in which the nucleus has an axisymmetric deformation, the rotational degrees of freedom are expected to play an important role at excitation energies around the neutron binding. In this case the collective enhancement factor can be promptly evaluated as

$$Z_{coll} = \sigma_{\perp}^2 = \frac{I_{\perp}}{\hbar^2} T. \quad (22)$$

A similar, simple, analytical expression can be derived also for nuclear excitations due to surface vibrations.

These prescriptions cannot be applied to the complete mass range. In fact, they assume the nucleus to have either rotational or vibrational degrees of freedom to be added to the intrinsic excitations. This classification is in many cases not possible.

A model which provides a unified description of collective properties of nuclear spectra is the Interacting Boson Model<sup>9)</sup>. Recently<sup>8)</sup>, this model has been applied for the evaluation of the collective enhancement factor  $Z_{coll}$ . However, the calculations made using this technique are still too involved to be enclosed into a simple recipe and in HERMES only the simple expression of Eq. (22) has been considered.

The relations given above have been coded into a computer program, HERMES, whose description and use will be given in the next chapter.

### 3. HERMES

#### 3.1 Introduction to HERMES

We will describe here the computer program HERMES. The program has been written in Fortran 77 and the source contains about 2000 records, excluding the *block-data* containing the experimental nuclear mass differences.

The program has been written in such a way that it runs interactively with the user. We will first describe its structure (section 3.2) and the various *menus* which are presented to the user while running it. At the mean time we will provide a brief description of the various physical assumptions made. The explanations on how to install the program, the description of the various files that the program uses and other technical details will be given in the sections 3.3 and 3.4.

The input/output of HERMES should be self-explanatory. We will give here the explanations for only a few examples of the various paths that can be followed when running HERMES. The name of variables or other quantities appearing in the program input/output will be given in a different type-style (like in *type-style*).

#### 3.2 Structure of HERMES

The structure of HERMES is shown in the flow-chart of Fig. 1. We give here a few examples of how the interactive procedure works. The program starts submitting the first menu:

```

Main Menu
-----
1) Start the calculation for a given isotope
2) Set/Reset defaults for the calculation
3) Build the systematics of LDP
99) STOP

```

As it is obvious, three selections can be made, in addition to the STOP (to end the execution).

Typing 1 the program will calculate the level density parameters for a single isotope. In this case the next request will be for the Mass number and Atomic number of the isotope under study.

To calculate the level density parameters, a certain number of options need to be specified. The program starts with all the possible options set to default values. To change and/or select options different from the defaults, the selection 2 in the main menu above should be made. For example, the calculation of the spin dispersion factor  $\sigma$  can be made assuming the nucleus to be spherical or deformed. Eq. (7) will be used in the former case and Eq. (10) in the

latter. The selection of one those two options can be made following the selection 2 in the main menu.

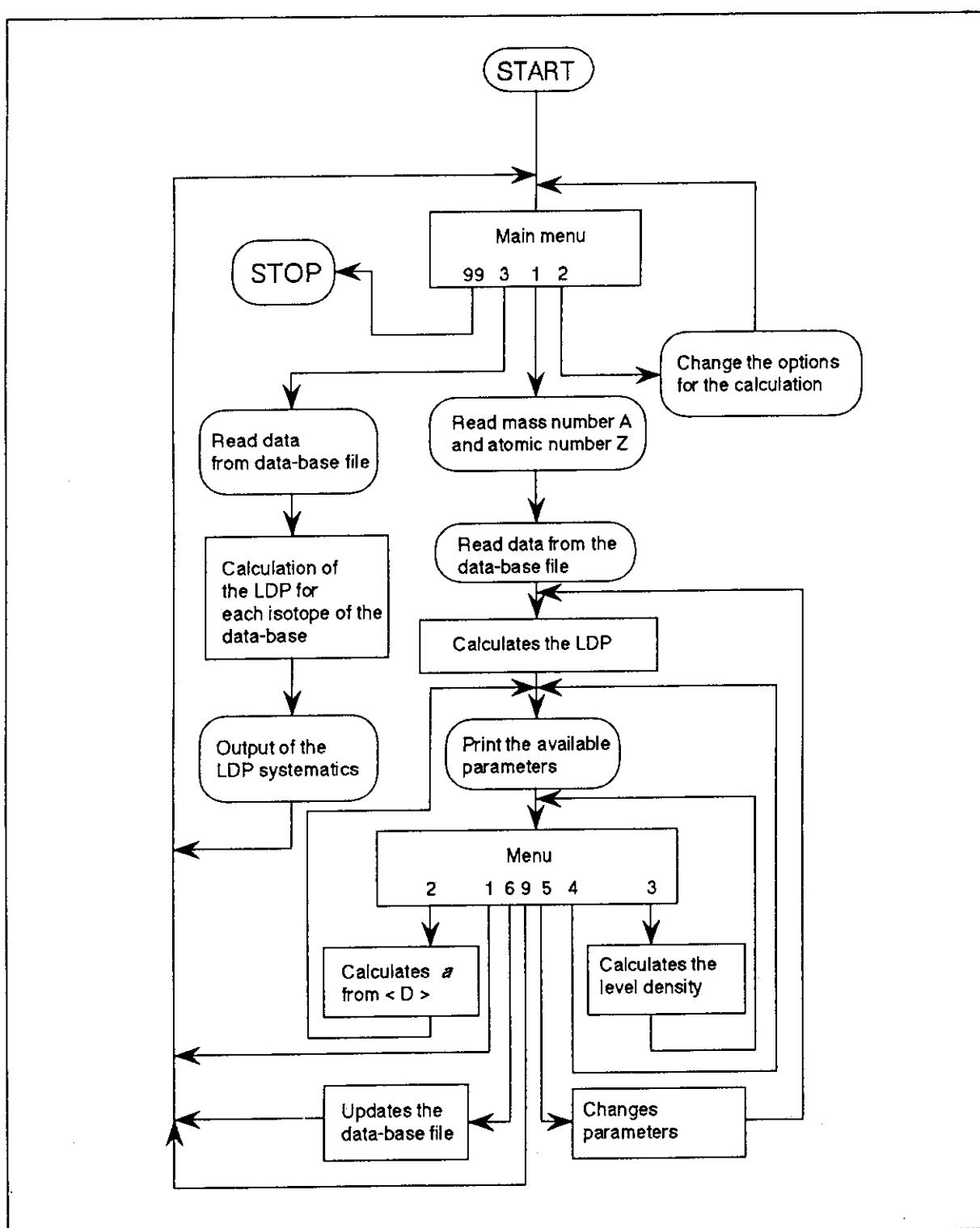


Figure 1. Flow-chart of HERMES.

Finally, typing 3 the program will construct the level density parameter systematics for all the nuclei contained in the data-base, using the options *currently* available.

If the selection 1 was to be made and the nuclear information are contained into the data-base file, the calculation of the level density parameters for the selected nucleus will be promptly performed. These includes the calculation of the spin dispersion factor  $\sigma^2$  ( sigma2 ), the shell correction energy  $E_{sh}$  ( Esh ) according to a specified liquid-drop mass formula, the level density parameters  $a(*)$  and  $a$ , the nuclear temperature  $T$  and so forth.

The resulting values will appear as

```
Parameters actually available:
**** 153Sm ****
Atomic number Z= 62    Neutron number N= 91
Target spin-parity      :      .0+
Neutron binding (Sn)   : 5.86737 MeV
En (above Sn)          : .00000 MeV
delta (back-shift)     : .97014 MeV
U (Sn+En-delta)       : 4.89722 MeV
Temperature             : .52312 MeV
Shell correction (Esh) : 3.67499 MeV
Deformation (Beta2)    : .00000
Zcoll (J=|It-1/2|)     : 1.00000
Zcoll (J= It+1/2 )    : 1.00000
sigma2                 : 31.80023
gamma                  : .07479 MeV**-1
a(*)-from systematics : 18.69185 MeV**-1
a                      : 22.99348 MeV**-1

Experimental <D(l=0)> : .05180 +/- .00330 KeV
Calculated   <D(l=0)> : .05961 KeV
              <D(l=1)> : .02050 KeV
```

Immediately after, the following menu will appear

```
Menu
1) Change Isotope
2) Calculate a and a(*) from given <D(l=0)>
3) Calculate the level density
4) Display available parameters
5) Change the parameters
6) Update the data-base file
9) Return
```

Selection 2 is particularly important because it provides the evaluation of the level density parameters that fit the experimental  $<D>_{l=0}^{exp}$ .

Selection 5 will give the user the opportunity to change individual parameters and repeat the calculations using the updated values. For example, if the user provides the value of the collective enhancement factor  $Z_{\text{coll}}$  evaluated using an independent technique, the evaluation of the level density parameters may be repeated taking into account of collective enhancement.

Finally, in Table 1 we give a list of the options that can be selected, if requested, selecting 2 in the main menu.

**Table 1** List of the options that can be selected in HERMES' main menu.

Heading	Selections	Action
Pairing (back-shift)	1*	pairing correction energy $\delta$ calculated according to Eq. (16)
	2	pairing correction energy $\delta$ as in selection 1 but with $\delta=0$ for odd-mass nuclei
	3	no pairing correction included
Mass formula	1*	Mass formula from Myers and Swiatecki <sup>10)</sup>
	2	Mass formula from Spanier and Johansson <sup>11)</sup>
	3	Mass formula from Möller and Nix <sup>12)</sup>
Nuclear deformation	1*	Deformation $\beta_2$ read on the data-base file
	2	Deformation $\beta_2$ calculated as in the reference <sup>11)</sup>
	3	Deformation $\beta_2$ calculated as in the reference <sup>13)</sup>
Damping parameter $\gamma$	1	constant
	2*	$\gamma = 0.40 / A^{1/3}$
	3	$\gamma = k / A^{1/3}$ , $k$ in input
Collective enhancement	1	$Z_{\text{coll}}$ calculated as in Eq. (22)
	else*	$Z_{\text{coll}} = 1$
Nuclear temperature	1	$T = (U/a)^{1/2}$
	2*	$T$ as defined in Eq. (13)
	3	$T$ calculated by numerically differentiating the total state density

\*default value.

There are two experimental mass-excess tables included in HERMES<sup>14)</sup>. In our previous work<sup>2)</sup> we have used the mass table from the CERN compilation. Here, we have used the more recent tabulation of Waspra et al.<sup>14)</sup>. This alternative choice resulted in a very small difference in the parameter systematics.

The routine that produces the mass difference is kept separated from the main program. In this way, each one of the two compilations, or any other additional mass compilation, can be readily incorporated into the program.

### 3.3 File allocation

HERMES requires the allocation of a maximum of three files. One contains the data-base of nuclear information required to calculate the level density parameters. This file is provided together with the computer program.

A second file allocation is required if a systematics of parameters is being constructed by the code. A version of this file, obtained using all-defaults for the calculation is given in Appendix A.

Finally, if the information for a given isotope is not contained in the data-base file or if it is contained but needs to be updated, a new version of the data-base file can be created by HERMES. This new version of the data-base file can be subsequently used as *input* data-base for further runs.

### 3.4 Installation

HERMES can be requested to the authors using the attached form (see Appendix B). The program and its files will be delivered in a diskette or through electronic-mail. In either case, the package will include:

- 1) the HERMES source program
- 2) a subroutine containing the experimental mass differences
- 3) a data-base file containing the nuclear structure information
- 4) the executable file for running HERMES on a personal computer (only in the diskette)

Independent compilers and linkers can be used to produce the executable file. We can provide the executable files compiled and linked using the Microsoft Fortran (ver 5.1), for either IBM (compatible) or NEC (compatible) personal computers.

The whole program has been divided into

```
-hermes.for
-mass.for
```

files (the source and the mass-excess block-data routine). They can be compiled and linked separately or merged first and then compiled and linked as a unique program.

In summary, the HERMES package contains:

Directory	Files	Contents
source	hermes.for	HERMES fortran source
mass	mass.for, mass.lib	mass-table ( Ref. <sup>14a)</sup> )
	newmass.for,newmass.lib	mass-table ( Ref. <sup>14b)</sup> )
exenec/exeibm	h.exe h8x87.exe	HERMES executable file HERMES executable file (math-coprocessor i8x87 required)
data	datab.dat	data-base file
	syst.dat	file containing the level density parameter-systematics
	updatab.dat	updated version of the datab.dat file
	startup.txt	mask text-file

## 4. EXAMPLES OF USE OF HERMES

### 4.1 Construction of the FGM parameter systematics

As an example of the use of HERMES we show here how to construct a level density parameter systematics using various options available in the program.

The construction of the nuclear level density parameter systematics has been performed several times in the past, perhaps the most quoted and recognized being those of Erba et al.<sup>15)</sup>, Lynn<sup>16)</sup> and Dilig et al. We have used the data on experimental nuclear level spacings  $\langle D \rangle_{l=0}^{\text{exp}}$  from the reference<sup>1)</sup> and then calculated the level density parameter  $a$  (selection 3 in the main menu of HERMES).

The results are shown in Figure 2. For clearness, a portion in a restricted region,  $100 \leq A \leq 200$ , is given separately.

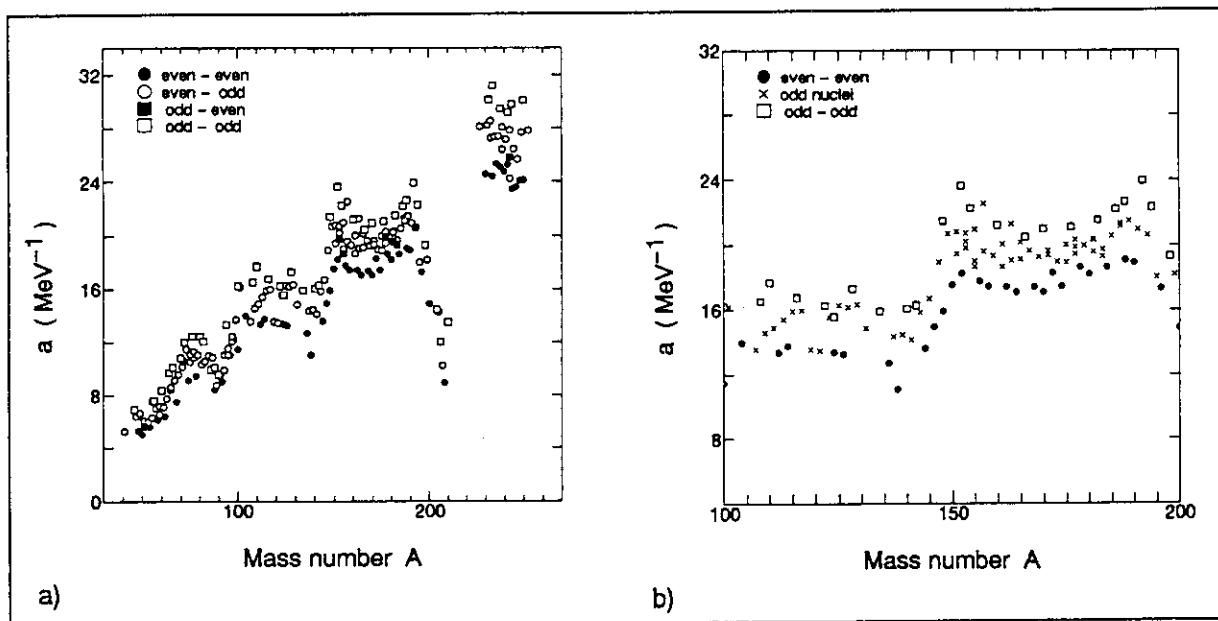
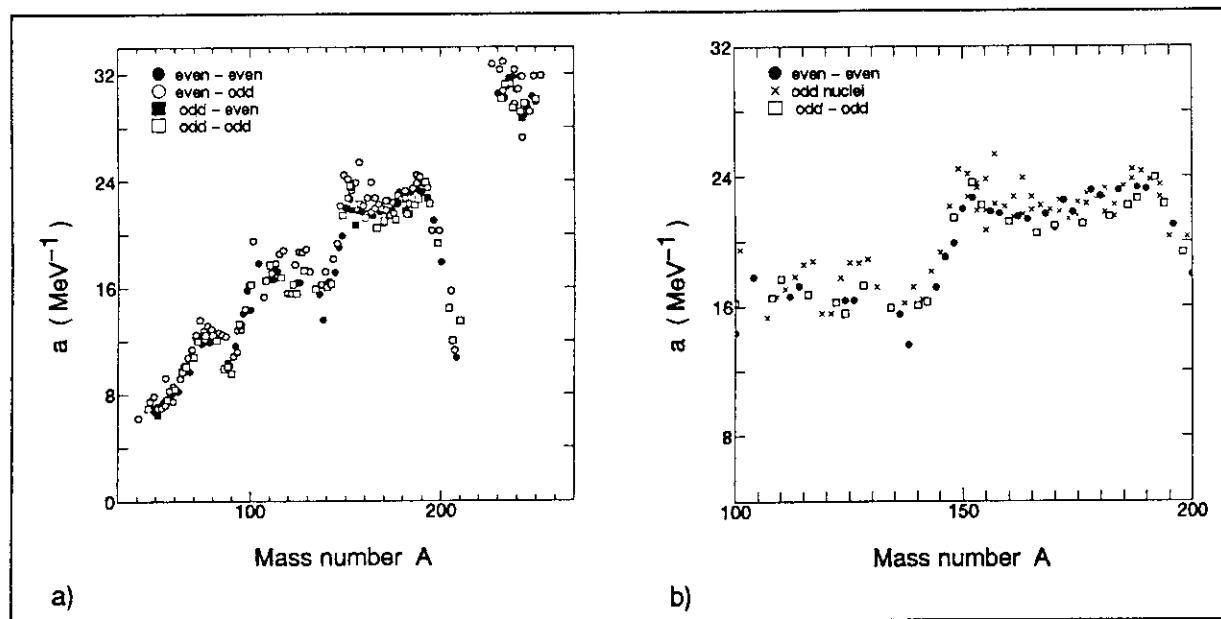


Figure 2. Level density parameter  $a$  from Eq. (2) for  $41 \leq A \leq 235$  (a) and for  $100 \leq A \leq 200$  (b).

In making Figure 2, no corrections to the FGM expressions were applied. However, as described in chapter 2, paring and shell effects can and should be incorporated into the FGM in order to have a more reliable parameter systematics.

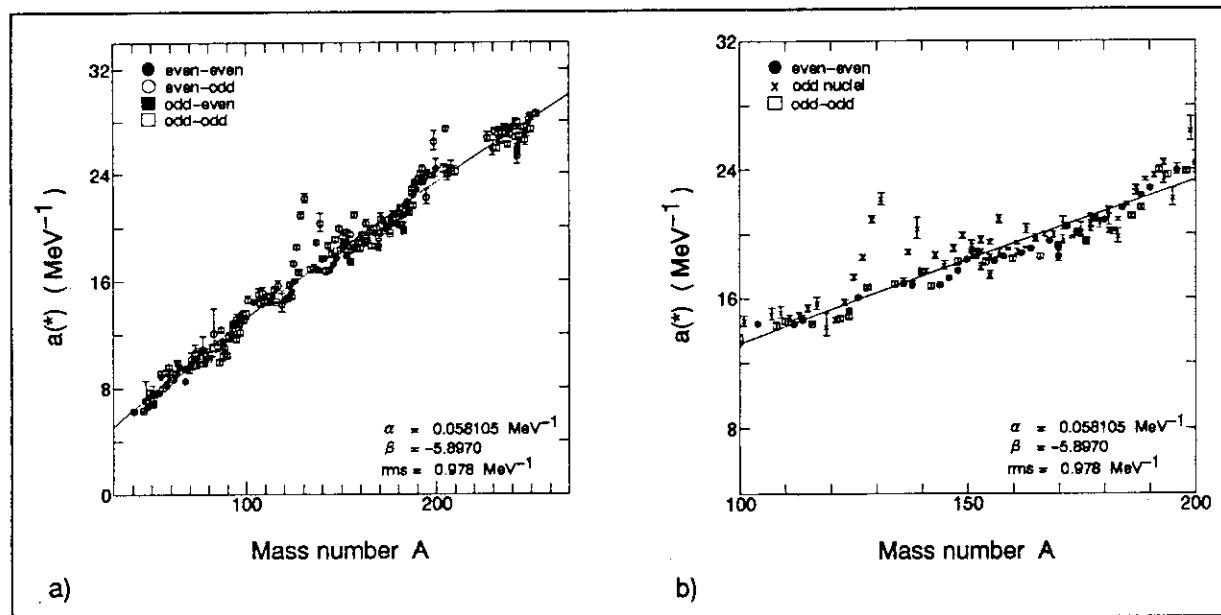
In fact, repeating the calculations made for Figure 2 and including the prescription of Eq. (16) to correct the FGM for pairing correlation effects, we have obtained Figure 3. As can be seen, the even-odd dependence of the  $a$ -parameter in the systematics is strongly reduced.



**Figure 3.** Level density parameter  $a$  from Eq. (2), with paring correction included, for  $41 \leq A \leq 235$  (a) and for  $100 \leq A \leq 200$  (b).

Shell effects are clearly present in the systematics of Figure 3. Using the technique described in 2.2, we have repeated the calculations for the nuclei in our data-base and built the systematics of the  $a(^*)$  parameter.

The results of the calculations are shown in Figure 4.



**Figure 4.** Level density parameter  $a(*)$  from Eq.(18) for  $41 \leq A \leq 235$  (a) and for  $100 \leq A \leq 200$  (b).

It clearly appears that the shell effects have, to a great extent, been appropriately taken into account by the procedure described above.

In Figure 4 we also show an evaluated "experimental" error associated to each  $a(*)$ . This is just the direct effect of the experimental uncertainties on  $\langle D \rangle_{l=0}^{\text{exp}}$ . The value of the damping parameter  $\gamma$  adopted in our calculation was<sup>17)</sup>

$$\gamma = \frac{0.40}{A^{1/3}} \quad \text{MeV}^{-1}. \quad (23)$$

The systematics of the  $a(*)$  parameter shown in Figure 4 can be well described by a smooth function of the mass number  $A$

$$a(*) = \alpha A(1 - \beta A^{-1/3}) \quad (24)$$

where the two parameters  $\alpha$  and  $\beta$  can be determined from a least-squares fit of the  $a(*)$  values. From the values plotted in Figure 4 we have obtained

$$\alpha = 0.058105 \quad \text{MeV}^{-1} \quad \text{and} \quad \beta = -5.8970 \quad (25)$$

with root mean square deviation,  $rms = 0.978 \text{ MeV}^{-1}$ .

This parametrization can be used to evaluate the level density parameters in the expression Eq. (2), for nuclei whose experimental information on the average level spacings is not available. In fact, from the value of  $a(*)$  obtained in Eq. (24), the level density parameter  $a$  can be calculated using Eq. (18) and the spin dispersion factor  $\sigma$  using Eq. (7) or Eq. (10).

For a more accurate analysis of our results, we have performed a least-squares fit to the  $a(*)$  calculated from the  $\langle D \rangle_{l=0}^{\text{exp}}$ , separately for nuclei of given even-odd character.

The results are summarized in Table 1. It can be noticed that the  $rms$  is smaller, compared to the global analysis, in three of the four sub-sets. This fact can allow a more accurate determination of the level density parameters for nuclei of unknown resonance spacings.

**Table 1** Parametrization of the  $a(*)$ -systematics according to Eq. (24).

nuclei	$\alpha$ (MeV $^{-1}$ )	$\beta$	$rms$ (MeV $^{-1}$ )	number of nuclei
all	0.058105	-5.8970	0.978	217
even-even	0.068072	-4.1136	0.567	51
even-odd	0.053127	-7.1799	1.090	112
odd-even	0.066794	-3.9051	0.767	8
odd-odd	0.065415	-4.4353	0.718	46

To have a better accuracy in the determination of the parameter  $a$ , a *local* systematics of  $a(*)$  should be constructed. In fact, the small fluctuation of  $a(*)$  in comparison with those of  $a$  allows for a much more reliable determination of this parameter and in turn for the level density at the neutron binding.

#### 4.2 Calculation of the level density parameters for a given isotope

An example of calculation of level density parameters for a given isotope has been given in section 3.2. In that case, the level density parameter  $a(*)$  for  $^{153}\text{Sm}$  was evaluated from the systematics constructed as described in the previous example. If one wants to calculate the level density parameters that fit the known experimental level spacings  $\langle D \rangle_{l=0}^{\text{exp}} = 51.8 \pm 3.3 \text{ eV}$ , one should select the option 2 in the menu shown in section 3.2. In this case the program will evaluate the level density parameter  $a(*)$  which is consistent with the measured level spacings and then it will calculate the other related parameters like the spin dispersion factor  $\sigma$ , the nuclear temperature  $T$ , and so forth. The results will appear as

Parameters actually available:		
<b>**** 153Sm ****</b>		
Atomic number Z= 62	Neutron number N= 91	
Target spin-parity	: .0+	
Neutron binding (Sn)	: 5.86737	MeV
En (above Sn)	: .00000	MeV
delta (back-shift)	: .97014	MeV
U (Sn+En-delta)	: 4.89722	MeV
Temperature	: .51943	MeV
Shell correction (Esh)	: 3.67499	MeV
Deformation (Beta2)	: .00000	
Zcoll (J= It-1/2 )	: 1.00000	
Zcoll (J= It+1/2 )	: 1.00000	
sigma2	: 31.57597	
gamma	: .07479	MeV**-1
a(*)	: 18.92682	MeV**-1
a	: 23.28252	MeV**-1
Experimental $\langle D(l=0) \rangle$	: .05180	+/- .00330 KeV
Calculated $\langle D(l=0) \rangle$	: .05180	KeV
$\langle D(l=1) \rangle$	: .01782	KeV

As one can see, there are small differences in comparison with the parameters shown previously. These are due to the difference between the value derived from the systematics and the valued derived from the experimental level spacings  $\langle D \rangle_{l=0}^{\text{exp}}$ .

## 5. CONCLUSIONS

We have described a well established technique to evaluate the FGM parametrization of nuclear level density at energies corresponding to the neutron binding energy. The model has been coded into a computer program, HERMES, which allows for the calculation of level density parameters. HERMES can be used as a stand-alone program as well as a part of a more general program for nuclear reaction calculations which uses the FGM prescriptions for the nuclear level density.

An example of application of HERMES has been given in which a parameter systematics for the nuclear level density has been constructed. Our parametrization can be easily incorporated into those computer codes that use the FGM prescriptions for the calculation of nuclear level densities. Our analysis included pairing correlations as well as shell inhomogeneities effects into the relations based on the FGM.

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## REFERENCES

- 1) Mughabghab S. F., Divadeenam M. and Holden N. E.: *Neutron Resonance Parameters and Thermal Cross Sections, Part A*, Academic, New York, (1981); Mughabghab S. F.: *ibid.*, Part B, Academic, New York, (1984).
- 2) Mengoni A. and Nakajima Y.: to be published in the *J. Nucl. Sci. and Techno.*, (1993).
- 3) The basic relations of the Fermi-Gas model level density have been derived in a number of papers and books (see Refs. 6,9) below). Perhaps, the most recent paper on the argument in which the basic relations given in the text are once more derived is: Engelbrecht C. A. and Engelbrecht J. R.: *Ann. Phys.*, **207**, 1 (1991).
- 4) See for example: Mengoni A., Fabbri F. and Maino G.: *Nuovo Cimento*, **94**, 297 (1986) and references therein.
- 5) See Ref. 16) below. For the BCS treatment see Maino G., Menapace E. and Ventura A.: *ibid.*, **A 57**, 427 (1980).
- 6) Bohr A. and Mottelson B. R.: *Nuclear Structure*, Vol. I, Benjamin, New York, (1969); *ibid.*, Vol. II, (1975).
- 7) Ignatyuk A. V., Istekov K. K. and Smirenkin G. N.: *Sov. J. Nucl. Phys.*, **29**, 450 (1979). For a recent review on the Generalized Superfluid Model see Rastopchin E. M., Svirin M. I. and Smirenkin G. I.: *ibid.*, **52**, 799 (1991); Ignatyuk A. V., Weil J. L., Raman S. and Kahane S.: *Phys. Rev.*, **C 47**, 1504 (1993).
- 8) Maino G., Mengoni A. and Ventura A.: *Phys. Rev.*, **C 42**, 988 (1990).
- 9) Iachello F. and Arima A.: *The Interacting Boson Model*, Cambridge University Press, (1987).
- 10) Myers W. D. and Swiatecki W. J.: *Nucl. Phys.*, **81**, 1 (1966).
- 11) Spanier L. and Johansson S. A. E.: *Atomic Data and Nuclear Data Tables*, **39**, 259 (1988).
- 12) Möller P. and Nix J. R.: *ibid.*, **39**, 213 (1988).
- 13) Raman S., Nestor Jr. C. W., Kahane S. and Bhatt K. H.: *ibid.*, **42**, 1 (1989).
- 14) a. CERN mass compilation: obtained by private communication to Fabbri F., ENEA, Bologna, (1981).  
b. Waspra A. H., Audi G. and Hoekstra R.: *Atomic Data and Nuclear Data Tables*, **39**, 281 (1988).
- 15) Erba E., Facchini U. and Saetta-Menichella E.: *Nuovo Cimento*, **22**, 1237 (1961).
- 16) Lynn J. E.: *The theory of neutron resonance reactions*, Clarendon Press, Oxford, (1968).
- 17) Ramamurthy V. S., Kataria S. K. and Kapoor S. S.: *Proceedings of the IAEA Advisory Group Meeting on Basic and Applied Problems of Nuclear Level Densities*, Brookhaven National Laboratory Report BNL-NCS-51694, 187, (1983).

## APPENDIX A

Here follows printout of the file containing the level density parameter systematics calculated by HERMES as described in the text.

This file contains the level density parameter systematics as constructed by the HERMES code.

Beta2	sigma**2									
	D(1=0)	err(D(1=0))	KeV	N	A	Spin	P	Z	Y	err(Y)
0.00000	45.00000	1	45.00000	6.00000	6.2083	-1104	-1276	6.2845	-1117	.1291
0.00000	1.30000	-1	1.30000	8.00000	6.9583	-0641	-0696	6.3039	-0581	.0631
0.00000	10.00000	-1	10.00000	4.00000	7.4595	-5420	1.6004	7.0656	-5134	.1159
0.00000	2.20000	-1	2.20000	3.00000	6.9146	-1449	-1763	6.5965	-1382	.1682
0.00000	13.00000	-1	13.00000	7.8437	7.2089	-2089	7.2684	7.6955	-2050	.2634
0.00000	125.00000	-1	5.00000	.50000	6.6417	-0859	0956	6.8764	-0890	.0989
0.00000	70.00000	-1	125.00000	7.0890	7.4789	-9352	7.2812	7.4919	.9606	-.3188
0.00000	6.00000	1	2.70000	6.4900	7.1962	-1962	6.7864	7.2054	.2723	-.6435
0.00000	15.00000	1	15.00000	2.00000	6.9648	-1098	-1267	7.5713	1.1194	.1378
0.00000	42.00000	1	29.50	5.00000	6.9833	-1074	1.1221	7.6564	-1117	.1339
0.00000	30.50	-1	7.10000	1.20000	7.4310	-1543	1.1852	7.6097	-.1580	.1896
0.00000	31.50	-1	26.00000	7.00000	9.2518	-3037	4.0892	8.9343	-.2932	.3942
0.00000	31.56	-1	2.70000	4.00000	7.6072	-1327	1.1556	7.9820	-.1392	.1633
0.00000	31.56	-1	13.00000	2.00000	7.1928	-1270	1.1270	9.1602	-.1617	.1908
0.00000	29.55	-1	17.00000	2.00000	8.2765	-1187	1.1348	9.2052	-.1321	.1499
0.00000	31.55	-1	17.00000	2.00000	8.2765	-1187	1.1348	9.2052	-.1321	.1499
0.00000	31.55	-1	6.00000	1.00000	7.9840	-1523	1.1822	8.3072	-.1585	.1896
0.00000	35.00000	-1	35.00000	15.00000	8.6192	-4192	1.6814	8.4278	-.4098	.6663
0.00000	1.10000	-1	1.10000	.10000	8.3994	-0884	0.974	8.7783	-.0924	.1018
0.00000	13.70000	-1	13.70000	2.00000	6.4652	-1252	1.1465	9.8582	-.1606	.1880
0.00000	16.00000	-1	16.00000	2.50000	8.3086	-1526	1.1805	9.1695	-.1684	.1992
0.00000	32.50	-1	1.80000	.30000	8.2193	-1495	1.1787	8.6896	-.1580	.1890
0.00000	33.50	-1	19.10000	3.60000	9.1820	-2063	2.5739	9.0701	-.2037	.2499
0.00000	33.60	-1	19.90000	3.60000	10.1697	-2242	2.2728	9.6064	-.2042	.2884
0.00000	33.60	-1	13.20000	.03000	9.7236	-0933	1.1031	9.8987	-.0950	.1049
0.00000	34.64	-1	11.4141	.73000	11.4141	-1649	1.1649	9.8824	-.1370	.1569
0.00000	34.64	-1	6.90000	1.00000	12.3558	-2077	1.2427	9.8249	-.1651	.1930
0.00000	35.65	-1	3.44000	.23000	9.9689	-0743	0.798	9.5875	-.0714	.0767
0.00000	4.70000	-1	4.70000	4.00000	10.7863	-1047	1.1147	9.4617	-.0919	.1006
0.00000	5.10000	-1	5.10000	0.2000	9.7021	-0420	0.0438	8.5135	-.0370	.0385
0.00000	5.77000	-1	5.77000	1.00000	11.4141	-1649	1.1649	9.8824	-.1370	.1569
0.00000	5.1000	-1	6.90000	1.00000	12.3558	-2077	1.2427	9.8249	-.1651	.1930
0.00000	35.65	-1	1.81000	.03500	10.8199	-1975	2.4256	9.3369	-.1702	.2091
0.00000	4.72	-1	2.25000	.04800	12.0095	-2460	3.0707	9.5884	-.1978	.2486
0.00000	4.73	-1	1.5243	.3477	1.4377	-6707	10.1304	0.0385	1.1978	.43137
0.00000	4.73	-1	13.6080	.04000	13.8233	-5118	1.8130	10.1618	-.3541	.5445
0.00000	4.74	-1	11.8233	.02000	11.8233	-2687	3.491	9.5912	-.2686	.2861











## APPENDIX B (request-form)

To obtain HERMES, please fill in and send the following form:

Name : \_\_\_\_\_

Institute : \_\_\_\_\_

Address : \_\_\_\_\_  
\_\_\_\_\_

I would like to receive a copy of the package HERMES through:

diskette (5.25")       diskette (3.5")       e-mail  
 IBM (or compatible) format       NEC (or compatible) format

Date \_\_\_\_\_

Please send to:

Dr. Yutaka NAKAJIMA

Nuclear Data Center

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319-11 Tokai-mura, Naka-gun

## Ibaraki-ken, JAPAN

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